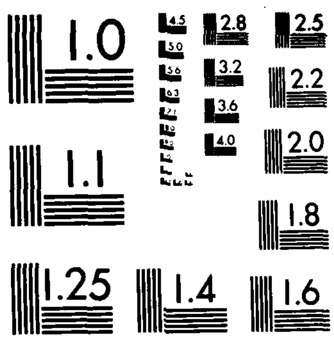
AD-A174 826 TRANSPORT PHENOMENA AND INTERFACIAL KINETICS IN MULTIPHASE COMBUSTION SYS (U) YALE UNIV NEW HAVEN CT HIGH TEMPERATURE CHEMICAL REACTION ENG D E ROSNER 1/1

UNCLASSIFIED JAN 85 AFOSR-TR-86-2044 AFOSR-84-0034 F/G 21/2 NL



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

AD-A174 826

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

(2)

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION unclassified	1b. RESTRICTIVE MARKINGS none
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for Public Release: Distribution Unlimited.
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR- 86-2044
6a. NAME OF PERFORMING ORGANIZATION YALE UNIVERSITY	6b. OFFICE SYMBOL (If applicable)
7a. NAME OF MONITORING ORGANIZATION AFOSR/NA	
6c. ADDRESS (City, State, and ZIP Code) High Temperature Chem. Engrg. Lab Chem. Engrg. Dept., Mason Lab, Rm. 319 9 Hillhouse Ave., New Haven, CT 06520	7b. ADDRESS (City, State, and ZIP Code) Bolling Air Force Base, D.C. 20332-6448
8a. NAME OF FUNDING/SPONSORING ORGANIZATION AIR FORCE OFFICE OF SCIENTIFIC RESEARCH	8b. OFFICE SYMBOL (If applicable) AFOSR/NA
9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER Grant AFOSR 84-0034	
8c. ADDRESS (City, State, and ZIP Code) Bolling Air Force Base, D.C. 20332-6448	10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.
-61102F-	-2308-	-A2-	

DTIC ELECTE DEC 5 1986

11. TITLE (Include Security Classification)
TRANSPORT PHENOMENA AND INTERFACIAL KINETICS IN MULTIPHASE COMBUSTION SYSTEMS (unclassified)

12. PERSONAL AUTHOR(S)
Rosner, Daniel E.

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
annual technical	FROM 12/1/83 TO 11/30/84	January, 1985	-12-

16. SUPPLEMENTARY NOTATION
... under the grant include (1)

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	aerosols, convective diffusion, deposition; energy transfer; catalysis; fouling; soot.
-21-	-01-		
-21-	-02-		

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This report summarizes Yale High Temperature Chemical Reaction Engrg. laboratory research methods/results (Grant AFOSR 84-0034) for the one-year period ending 11/30/84. Research accomplishments include (1) the demonstration of several laser-based real-time optical techniques for measuring vapor-particle-deposition rates onto cooled surfaces in combustion gases; (2) demonstration that thermophoresis dominates the capture of soot particles by thermocouples in laminar flames and that this phenomenon can be exploited to infer both local soot volume fractions and local gas temperatures; (3) development of effective boundary layer computational methods and correlations for thermophoretically-modified small particle transport across laminar and turbulent boundary layers; and (4) extension of the recently developed microwave induced plasma emission spectroscopic (MIPES) method to follow boron surface gasification kinetics. Seven presentations and eight publications describing these techniques/findings are documented. Keywords: Aerosols; Convective diffusion

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT ☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED
22a. NAME OF RESPONSIBLE INDIVIDUAL Dr. Julian Tishkoff	22b. TELEPHONE (Include Area Code) (202) 767-4935
22c. OFFICE SYMBOL AFOSR/NA	

DD FORM 1473, 84 MAR — 83 APR edition may be used until exhausted. All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE
UNCLASSIFIED

DTIC FILE COPY

412367-SH

AFOSR-TR- 86-2044

January, 1985

ANNUAL TECHNICAL REPORT

Approved for p... release; distribution unli...ted.

to

U.S. AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
Bolling Air Force Base
Washington, D.C. 20332-6448

Grant AFOSR 84-0034

TRANSPORT PHENOMENA AND INTERFACIAL KINETICS IN MULTIPHASE COMBUSTION SYSTEMS

Principal Investigator: Daniel E. Rosner

Period Covered: 1 December 1983 - 30 November 1984

High Temperature Chemical Reaction Engineering Laboratory
Yale University
Department of Chemical Engineering
P.O. Box 2159 Yale Station
New Haven, CT 06520

APPROVED FOR PUBLIC RELEASE: DISTRIBUTION UNLIMITED

QUALITY INSPECTED 4

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH (AFSC)
NOTICE OF TRANSMITTAL TO DTIC
This technical report has been reviewed and is approved for public release IAW AFR 190-12.
Distribution is unlimited.
MATTHEW J. KERPER
Chief, Technical Information Division

A-1

The views and conclusions cont.ined in this document are those of the authors and should not be interpreted as necessarily the official policy or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U. S. Government.

86 12 04 041

1. INTRODUCTION

The performance of gas turbine (GT) engines in dusty atmospheres or at very high turbine inlet temperatures, or when using jet fuels from non-traditional sources (e.g., shale, or coal-derived), and the performance of ramjets burning slurry fuels leading to condensed oxide aerosols, will depend upon the formation and transport of small particles across non-isothermal combustion gas boundary layers. Moreover, even engines burning "clean" fuels can experience soot formation/deposition problems, including combustor liner burnout, and accelerated turbine blade erosion and "hot" corrosion. Accordingly, our research is directed toward providing design engineers with quantitative information on important gas/liquid and gas/solid rate processes at high temperatures.

An interactive experimental-theoretical approach is used to gain an understanding of and develop rational engineering correlations for performance-limiting chemical, and mass/energy transfer phenomena at interfaces. This includes the development and exploitation of laboratory flat flame burners (Fig. 1), and flow-reactors, along with novel diagnostic techniques. Resulting experimental data, together with the predictions of comprehensive asymptotic theories, are then used as the basis for proposing and verifying simple viewpoints and effective engineering correlations.

The purpose of this report is to briefly summarize our research methods and accomplishments under AFOSR Grant 84-0034 (Technical Monitor: J. M. Tishkoff) during the one-year period: 12/1/83 - 11/30/84. Readers interested in greater detail than that contained in Section 2 are advised to consult the published papers cited in Section 2. Copies of any of these published papers or preprints can be obtained by writing the PI: Prof. Daniel E. Rosner at the Department of Chemical Engineering, Yale University, Box 2159 Yale Station, New Haven, CT, 06520, U.S.A. Comments on, or examples of, the applicability of our research results will be especially welcome.

2. RESEARCH ACCOMPLISHMENTS AND PUBLICATIONS

Most of the results we have obtained under Grant AFOSR 83-0034 can be subdivided into the three sections below:

2.1 Particle Mass Transfer Experiments

The dominant role of thermophoresis (particle drift down a temperature gradient) in determining the deposition rate of submicron particulate matter from combustion gases[1,2], has recently been demonstrated in our laboratory by using four independent "real-time" experimental methods:

1. small thermocouple (TC) response to the amount of deposit[3]
2. laser-reflectivity (LR) of deposition target
3. laser-scattering from surface deposit (LSSD)
4. laser-extinction by the surface deposit (LESD)

the second of which is fully described in a paper on submicron MgO-particle deposition[4]. Methods 1, 3 and 4 have been illustrated for combustion systems yielding carbonaceous soot. All techniques applied to date have been under conditions of low particle mass loading[1], and negligible particle inertia[5].

Undoubtedly the simplest to implement is that based on the response of a thermocouple in a "dusty gas". For example, when a TC bead is immersed in soot-laden combustion products (say, downstream of a water-cooled flat-flame burner) soot deposition mass fluxes can be inferred photographically, as well as estimated *via* a quasi-steady energy balance and the TC bead's thermal response to the growing deposit (Fig. 2). Our results have been compared to a theory of particle thermophoresis in the gas thermal boundary layer (BL) surrounding the TC target; a theory which suggests straight line plots (Fig. 3) whose slope should be proportional to the local soot volume fraction. When the TC bead is immersed in a series of different soot-laden flames its response indeed correlates with the flame soot-loading, as inferred *via* our *in situ* laser beam extinction measurements. We have concluded that:

a) observed soot deposition mass fluxes are several orders-of-magnitude greater than those expected based only on Brownian (concentration) diffusion at the prevailing Reynolds numbers,

b) knowing the particle size-insensitive thermophoretic diffusivity, the local soot loading can be obtained *via* the slopes of linear plots (cf. Fig. 3) constructed exclusively from our experimental thermocouple temperature response information. Accordingly, this technique should be useful in probing three-dimensional combustor flows, in which the application of line-of-sight laser techniques is inadequate,

c) the dependence of soot deposition rates on the temperature "contrast" between the gas and target is in accord with proposed thermophoretically dominated mass transport theory (cf. straightness of data points in Fig. 3),

d) the behavior of submicron soot particles in non-isothermal combustion products is strongly influenced by thermophoresis, with important implications for understanding rates of soot nucleation, growth, coagulation, burnout and deposition.

We have just developed two new laser probe methods based on either the measurement of light intensity *scattered* from or extinguished by particles depositing on an immersed transparent gas-cooled (back side) sapphire disk (Fig. 1). These methods, which we find to be extremely sensitive to the amount of material deposited, enable us to study the effects of thermophoresis at T_w/T_e-values much lower than 0.7 (previously studied using our reflective Pt-ribbon targets (method 2)). Although these experiments are in progress, our preliminary evidence for soot acquisition on the target surface is consistent with the abovementioned conclusions concerning the dominance of thermophoretic particle transport.

Our earlier use of reflected laser light interference to monitor in real-time B_2O_3 deposition from the vapor phase (seeded combustion products) has just appeared in print[16].

2.2 Mass Transfer Theory

The understanding, prediction and correlation of vapor and particle mass transport across laminar and turbulent wall boundary layers (e.g., turbine blades (Fig. 4a) or combustor can walls) and mixing layers has motivated our recent research on boundary layer theory under conditions of non-Fickian mass

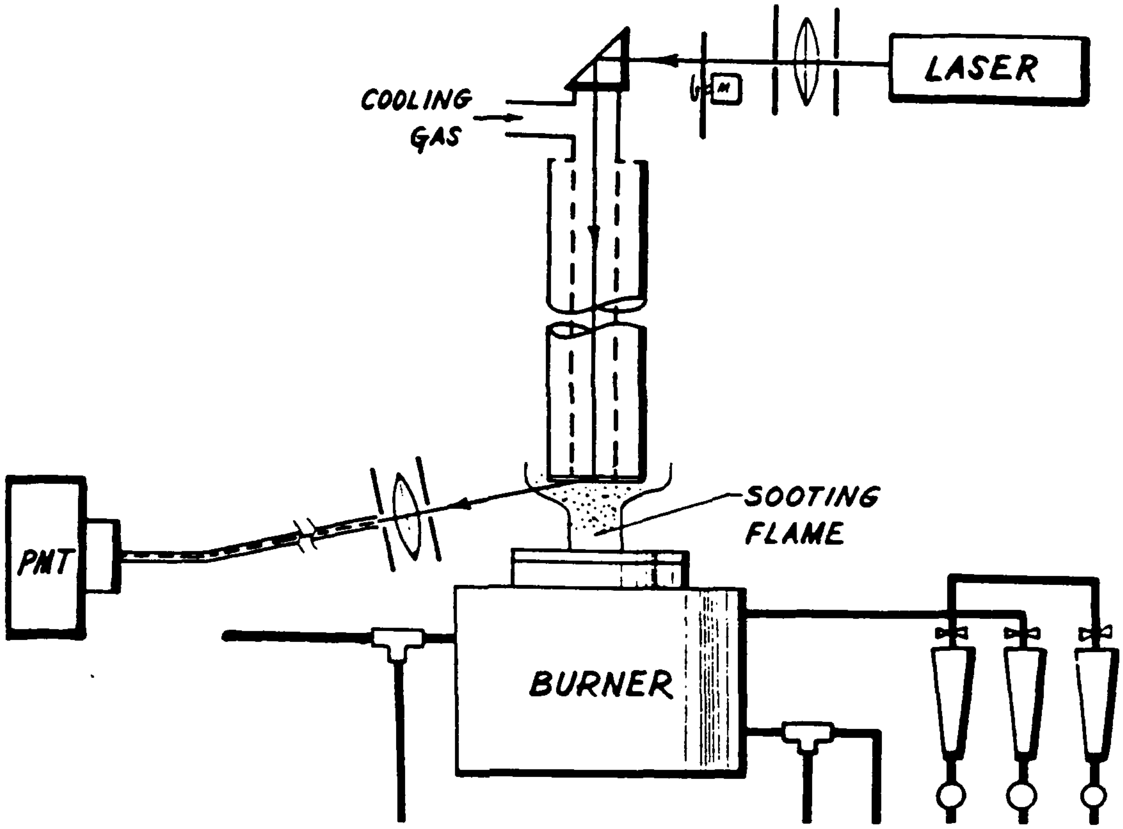


Fig. 1: Atmospheric pressure flat flame water-cooled burner, showing gas-cooled probe for particle deposition studies via laser light scattering (from the deposit)[3].

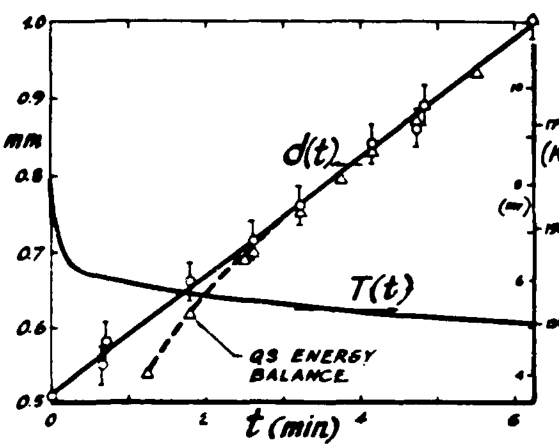


Fig. 2: Diameter and temperature response of a thermocouple junction inserted into a soot-containing flame.[3]

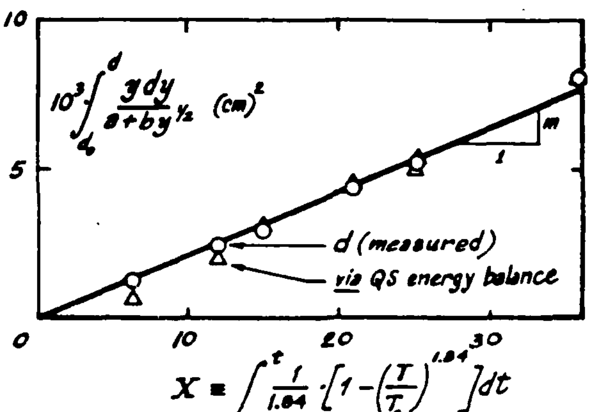


Fig. 3: Straight line plot for testing the dependence of soot deposition rate on surface- and gas-temperature.[3]

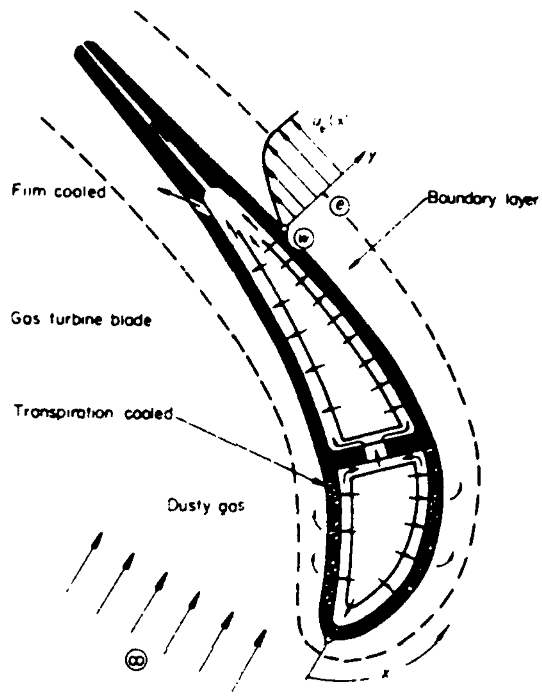


Fig. 4a: Configuration and station nomenclature. Transpiration-cooled and film-cooled turbine blade immersed in a high velocity, hot 'dusty' gas stream.

transfer[1]. Particularly important in combustion systems containing species of disparate molecular weight, is mass transfer driven by temperature gradients[1]; i.e., Soret diffusion (for vapors) and thermophoresis (for particles)[2]. Our initial investigations in the area were concerned with the effects of thermophoresis on forced-convective mass transport across laminar boundary layers[6] (including effects of variable thermophysical fluid properties and viscous dissipation). More recently, we have investigated the large effects of wall transpiration cooling for both laminar and turbulent boundary layers (see below). An important outcome of this research has been a rational correlation procedure[7] which allows accurate engineering predictions of mass transfer coefficients (e.g., mass transfer Stanton numbers, St_m) in such systems, without repetitive recourse to expensive computer programs, or even more expensive experiments.

Some illustrative predictions for the important case of turbulent dusty gas boundary layers on impermeable and on transpiration-cooled surfaces[8] are included here*. For impermeable surfaces (cf. Fig. 4b) even the slightest temperature contrast (e.g., wall temperature only one percent less than mainstream temperature) is associated with order-of-magnitude increases in the convective mass transfer coefficient for particles with Schmidt numbers greater than 10^5 (ca. $d_p \geqslant 0.2\ \mu m$ particles). However, thermophoresis reduces, but by no means eliminates, the fouling rate protection offered by transpiration using a dust-free cooler gas (cf. Fig. 4c). This "effusion" technique can therefore be used to minimize particle deposition within cooled combustion gas sampling probes.

2.3 Heterogeneous Kinetics

To make (i) instantaneous gas/solid reaction rate measurements over a large temperature range in a single experimental run, and (ii) surface mass balances necessary for mechanistic understanding of high temperature gas/solid reactions,[15] we have recently been exploiting an emission spectroscopic technique[9] developed, in part, under F49620-82K-0020. In this technique, a low-pressure microwave-induced plasma (MIP) excites characteristic emission from the atoms in the gaseous product species of a gas/solid reaction in a low pressure flow reactor.

We employ a modified version of the transonic, vacuum flow reactors (Fig. 5) developed earlier under AFOSR-support for the study of gas/solid reactions by Rosner and co-workers[10-12]. However, now the reaction product vapor species are dissociated and electronic emission from the resulting atoms is produced in a second microwave discharge plasma (G) before leaving the reactor. Evaporation and gasification reactions are studied by measuring emission intensity from this discharge, via a quartz window, a 75 mm-focal-length condensing lens and a 0.5m Jarrell-Ash monochromator.

Aside from steady-state reaction rate measurements, flash evolution experiments can be carried out to measure the amount of condensed product

* The parameter $\alpha_T Le$ appearing in Figs. 4b,c is the ratio of the particle thermophoretic diffusivity ($\alpha_T D_p$) to the heat diffusivity of the carrier gas mixture. According to kinetic theory, for particles small compared to the prevailing mean-free path, this ratio is near 0.4 and, remarkably, particle size insensitive.

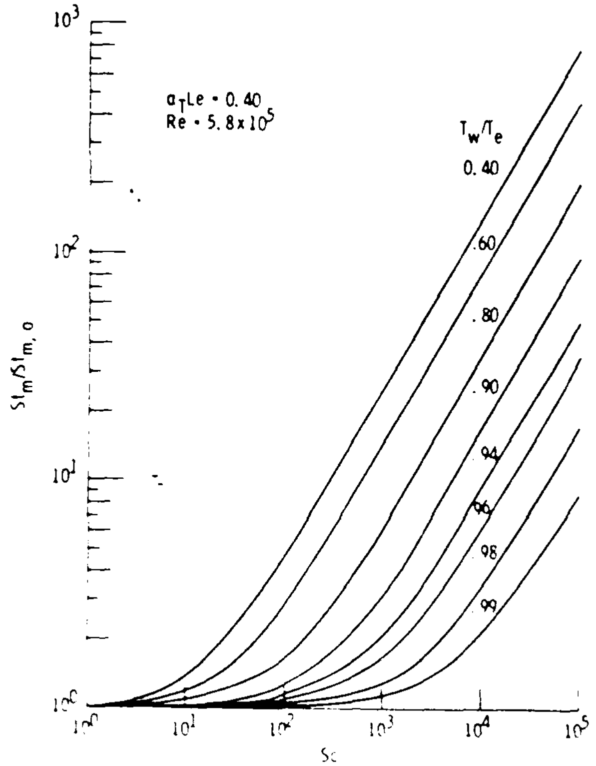


Fig. 4b: Schmidt-number dependence of thermophoretic mass transfer augmentation factor for various cold solid wall TBL conditions.[8]

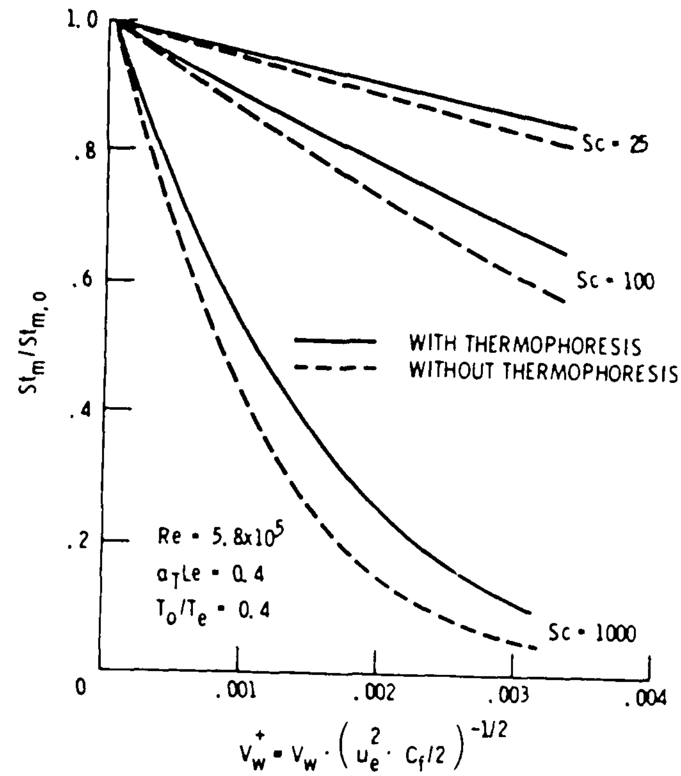
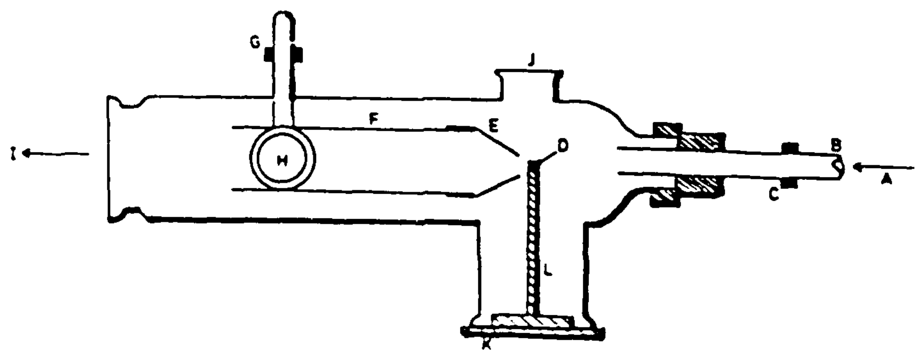


Fig. 4c: Deposition rate reduction due to transpiration cooling for a turbulent boundary layer.[8] Effect of thermophoresis in offsetting the fouling rate advantages of transpiration as a function of blowing rate and Schmidt number (particle size).



A, reactant and inert gas mixture. B, alumina tube. C, microwave cavity. D, electrically heated specimen filament; E, aluminum skimmer. F, pyrex annular tube; G, microwave cavity; H, quartz observation window; I, to pump, manometer, and throttle valve. J, pyrometer sight tube; K, specimen probe; L, electrical leads and voltage taps to measure specimen resistance.

Fig 5: Transonic flow reactor for kinetic studeis of gas/solid (filament) surface reactions using the method of microwave-induced plasma emission spectroscopy (MIPES)[9].

material formed on a surface during reaction, provided, of course, that the reaction product has a higher volatility than that of the substrate. In such experiments the filament is exposed to the gaseous reagent for some reaction time (normally only a few minutes). Then, the gaseous reagent flow into the reactor is stopped and the filament cooled to near 300K. Finally, the I(t) is determined when the filament is heated rapidly. The skimmer and the inner co-axial tube shown in Fig. 5 were installed so that the system detects only products from the central, uniform-temperature region of the filament. Valves are provided to divert the gaseous reagent to the reactor exhaust or to allow it to pass through the reactor during such "flash evolution" experiments.

Exploratory flash evolution experiments have been carried out for the F(g)/Pt(s) system[9] to demonstrate the capability of MIPES to rapidly and quantitatively follow low metal fluxes. We are now performing preliminary experiments on the application of this MIPES-technique to the oxidation of <u>boron</u>, a system of considerable interest to the propulsion community, but one whose poorly understood kinetics are apparently influenced by the condensibility of the reaction product B_2O_3.

Our earlier experiments on the use of <u>calorimetric techniques</u> to study the kinetics of heterogeneous reactions have been completed and prepared for publication in the cases of: a) energy accommodation for hydrazine decomposition[13] and b) surface-catalyzed combustion of hydrogen[14].

3. ADMINISTRATIVE INFORMATION, PERSONNEL

Table 3-1 summarizes the personnel who have contributed to this research program during the period: 12/1/83 - 11/30/84, along with subject matter of each investigator's research contribution. With the exception of our summer research assistant (S. Ogen) and A. Oner, whose work (Section 2.3) remains to be prepared for publication, these individuals comprise the PI's co-authors for the papers listed in Section 4.

TABLE 3-1
Summary of Personnel and their Contributions

NAME	STATUS @ YALE U.	PRIMARY CONTRIBUTION
Rosner, D.E.	PI[a], Fac. (ChE)	Overall program direction
Castillo, J.	PDRA	(BL) theory of particle transport
Eisner, A.D.	PDRA	Soot-particle deposition rate experiments[3]
Fernandez de la Mora, J.	Fac. (ME)	BL theory of particle transport[5]
Garcia-Ybarra, P.	PDRA (8/84)	Thermophoretic coefficient of nonspherical particles
Halpern, B.	Fac. (ChE)	Chemical and physical energy accommodation[13]
Liang, B.	GRA (85)	Vapor deposition in BL phase change
Nagarajan, R.	GRA (85)	BL theory of chemical vapor deposition[17]
Ogen, S.	SRP[d]	Soot particle deposition rate experiments[3]
Oner, A.	GRA/PDRA (85)	Microwave-induced plasma emission spectroscopy for boron gasification[9]
Park, H.M.	GRA (87)	BL theory of particle deposition
Quinlivan, G.	SRP	BL theory with vapor nucleation

[a] Principal Investigator
[b] Graduate Research Assistant (year of Ph.D. degree)
[c] Postdoctoral Research Assistant
[d] Summer Research Program, Yale Engineering and Applied Science

TABLE 3-2
Summary of Talks Based in Part on OSR-Grant

DATE	LOCATION	TOPIC
3/3/84	Yale U.	ChE Aspects of Chemical Vapor Deposition (CVD) Processes
3/12/84	General Motors Research Lab	Deposition from Combustion Gases
6/6/84	Amsterdam, Netherlands	Particle Mass Transfer Across Turbine Blade Boundary Layers (29th Int. Gas Turbine Conf.)
6/19/84	OSR Boron Combustion Workshop	Flow Reactor Studies of the Kinetics of Heterogeneous Boron Gasification Reactions
6/21/84	Pittsburgh, PA	Particle and Mass Transport Through Nonisothermal Combustion Gases (OSR/ONR Contractors Mtg.)
7/25/84	Wolfboro, NH	CVD Consequences of Vapor Phase Boundary Layer Phenomena (Gordon Research Conf.; High Temperature Chemistry)
11/30/84	Livermore, CA	Deposition from Combustion Gases (Sandia Labs)

4. REFERENCES

1. Rosner, D.E., J. PhysicoChemical Hydrodynamics 1, 159-185 (1980).

2. Rosner, D.E. and Fernandez de la Mora, J., ASME Trans.-J. Engrg. for Power 104, 885-894 (1982).

3. Eisner, A.D. and Rosner, D.E., "Experimental Studies of Soot Particle Thermophoresis in Non-Isothermal Combustion Gases Using Thermocouple Response Techniques," Combustion and Flame (submitted, 1984); see also, "Experimental and Theoretical Studies of Submicron Particle Thermophoresis in Combustion Gases," J. PhysicoChem. Hydrodynamics (in press, 1985).

4. Rosner, D.E. and Kim, S.S., "Optical Experiments on Thermophoretically Augmented Submicron Particle Deposition from 'Dusty' High Temperature Gas Flows," The Chemical Engineering J. 29, 147-157 (1984).

5. Fernandez de la Mora, J. and Rosner, D.E., J. Fluid Mechanics 125, 379-395 (1982); see also, Rosner, D.E. and Fernandez de la Mora, J., "Boundary Layer Effects on Particle Impaction and Capture," ASME-J. Fluids Engrg. 106, 113-114 (1984).

6. Gokoglu, S.A. and Rosner, D.E., "Thermophoretically-Augmented Forced Convection Mass Transfer Rates to Solid Walls Across Non-Isothermal Laminar Boundary Layers," AIAA J. (in press, 1985); see also, Gokoglu, S.A., Thermophoretically-Enhanced Deposition of Particulate Matter Across Nonisothermal Boundary Layers, Ph.D. Dissertation, Yale U., Chem. Engrg. Dept. (1982).

7. Gokoglu, S.A. and Rosner, D.E., "Correlation of Thermophoretically-Modified Small Particle Diffusional Deposition Rates in Forced Convection Systems with Variable Properties, Transpiration Cooling and/or Viscous Dissipation," Int. J. Heat Mass Transfer 27, 639-645 (1984); see also, Rósner, D.E., Gokoglu, S.A. and Israel, R., In Fouling of Heat Exchanger Surfaces, R. Bryers, Ed., Engrg. Foundation, NY, 235-256 (1983).

8. Gokoglu, S.A. and Rosner,D.E., "Thermophoretically Enhanced Mass Transport Rates to Solid and Transpiration-Cooled Walls Across Turbulent (Law-of-the-Wall) Boundary Layers," I/EC Fundamentals (in press, 1985); see also, Gokoglu, S.A. and Rosner, D.E., Int. J. Heat Fluid Flow 5, No. 1, 37-41 (1984).

9. Oner, A., Application of Microwave-Induced Emission Spectroscopy to the Study of Gas/Solid Surface Reaction Kinetics, Ph.D. Dissertation, Yale Univ., Dept. of Chemical Engineering (in preparation, 1984).

10. Rosner, D.E. and Allendorf, H.D., J. Phys. Chem. 75, 308-317 (1971).

11. Nordine, P.C. and Rosner, D.E., J. Chem. Soc., Faraday Trans. I 72, 1526-1533 (1976).

12. Nordine, P.C., Rosner, D.E. and Kindlmann, P.J., Rev. Sci. Instrum. 44, 821-826 (1973).

13. Kiela, J.B., Halpern, B.L. and Rosner, D.E., "Chemical and Physical Accommodation in the Metal-Surface-Catalyzed Decomposition of Hydrazine Vapor," J. Phys. Chem. 88, 4522-4527 (1984).

14. Israel, R., Thermal Diffusion Effects on Fuel Vapor Mass Transport Across Non-Isothermal Boundary Layers in Surface Catalyzed Combustion, Ph.D. Dissertation, Yale Univ., Dept. of Chemical Engineering (1983).

15. Rosner, D.E., AIAA J. 2, 593-610 (1964).

16. Seshadri, K. and Rosner, D.E., "Optical Methods and Results of Dew Point and Deposition Rate Measurements in Salt/Ash-Containing Combustion Gases -- $B_2O_3(\ell)$ Deposition Rates by Interference Method and Comparisons with Theory," Amer. Inst. Chem. Engrg. J. 30, No. 2, 187-196 (1984).

17. Rosner, D.E. and Nagarajan, R., "Transport-Induced Shifts in Condensate Dew Point and Composition in High Temperature Multicomponent Systems with Chemical Reaction," Chem. Engrg. Science (in press, 1985).

END

1-87

DTIC